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IN STRUCTURAL MECHANICS

Calibration of constitutive models with error control

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Abstract

In this thesis a framework for the calibration of constitutive models is presented. The framework involves the formulation of an optimization problem which is solved using strategies based on, essentially, Newton's method. The introduction of an additional costate field in order to incorporate the state equation has the advantage that error control in an arbitrary "goal" quantity is formally straightforward. The errors analyzed are those that arise from the Finite Element discretization and from uncertainties in the experimental data. Among the applications, moisture transport in wood and nonlinear viscoelasticity are discussed in more detail.

Keywords: Parameter identification, Calibration, a posteriori error estimation

Insensibly one begins to twist fact to suit theories, instead of theories to suit facts.

Sherlock Holmes / Sir Arthur Conan Doyle

Preface

The work presented in this thesis was carried out during the years 2003-2007 at the Department of Structural Engineering and Mechanics (2003-2004) and the Department of Applied Mechanics (2005-2007). This research was financially supported by the Swedish Foundation for Strategic Research (Project Computational Mathematical Modeling: Chalmers Finite Element Center), the Swedish Research Council (Project Global Calibration of Constitutive Models via Optimization and Sensitivity Assessment with Automatic Error Control), the National Graduate School for Scientific Computing (NGSSC) and special funding from the Dean of the School of Civil Engineering. All the support is most gratefully acknowledged.

First of all, I would like to express my deepest and sincerest gratitude to my supervisor and examiner Professor Kenneth Runesson for his enthusiasm, broad knowledge and open door. Also, I would like to thank my co-supervisor Dr. Fredrik Larsson for his helpfulness, clever ideas and valuable suggestions. In addition, I would like thank my other coauthors: Dr. John Eriksson, Dr. Jonas Danvind (Valutec AB) and Dr. Lars Nordström for our fruitful collaboration.

My colleagues, former as well as present, have been a very good support and have created a very nice atmosphere (also after working-hours). In particular, the "ByggMek" and "NäraHem" groups have provided me with a more realistic view of the world.

Finally I would like to thank Maria, my friends, and my family for their love and support, and for constantly reminding me that work isn't everything.

Göteborg, August 2007
Håkan Johansson

Thesis

This thesis consists of an introduction and the following appended papers:

Paper A H. Johansson, K. Runesson and F. Larsson. Parameter identification with sensitivity assessment and error computation. *GAMM Mittelungen* **30**, 430–457 (2007).

Paper B J. Eriksson, H. Johansson and J. Danvind. Numerical determination of diffusion coefficients in wood using data from CT-scanning. *Wood and Fiber Science* **38**, 334–344, (2006).

Paper C H. Johansson and K. Runesson. Calibration of a class of nonlinear viscoleasticity models with sensitivity assessment based on duality. *International Journal for Numerical Methods in Engineering* **69**, 2513–2537, (2007).

Paper D H. Johansson, K. Runesson and F. Larsson. Calibration of a class of nonlinear viscoelasticity models with adaptive error control. Published online in *Computational Mechanics*, doi: 10.1007/s00466-007-0172-z (2007).

Paper E H. Johansson, F. Larsson and K. Runesson. Estimation of model errors in the calibration of viscoelastic material models. To be submitted for publication

The appended papers were prepared in collaboration with the co-authors. The author of this thesis was responsible for the major progress of work in Papers A, C-E, i.e. was the prime responsible in planning the papers, took part in developing the theory, developed the numerical implementations and carried out the numerical simulations. In Paper B, a joint part was taken in the theoretical and numerical developments.

Contents

Introduction to the thesis

1 Introduction

As numerical simulations have become an integral part of modern engineering practice, the reliability of the simulation results hinges critically on the (lack of) knowledge regarding input parameters (loading, initial and boundary conditions, material parameters, etc.), in addition to (and, in fact, to a larger extent than) the quality of the solution algorithm itself, including the proper choice of FE-discretization. Some of the input parameters are in the general case determined indirectly from experiments by the solution of a nonlinear Least-Squares problem, whereby the sought parameters give optimal fit between predicted (computed) and measured response.

Although considerable attention has been paid to the analysis and solution of inverse problems, a rather limited amount of work has been devoted to the error estimation (from discretization and other sources) for this class of problems. In fact, the different errors are intertwined in the following way: The computation of the predicted response for a given model and numerical algorithm is marred by different errors, stemming from, e.g., discretization of the mathematical model, inexact modeling of the constitutive behavior (model error), simplified description of the experimental setup, and other numerical errors (round-off, pre-set tolerances etc.). Since the inverse problem involves the computation of the predicted response, all the mentioned model and numerical errors will be carried over to the solution of the inverse problem, i.e. there will be a resulting error in the obtained parameters. As the inverse problem has the additional complication of being ill-posed in the general case, the errors can be significantly amplified, and it is therefore essential that the reliability ("quality") of the solution to the inverse problem is determined. An additional important source of error is measurement errors, which are often present in terms of noise. In this thesis, we will discuss methods for the estimation of the inherent sources of errors.

1.1 Scope and delimitation

The scope of the present thesis is to extend a previously developed method for a posteriori computation of discretization errors to parameter identification problems. In particular, we try to obtain tools to determine to what extent the solution to an identification problem can be trusted. Hence, the focus is on the methodology and its application to somewhat academic examples, rather than on specific engineering applications (although one such application is the topic of paper B). Another important delimitation is that we here focus on the analysis of the obtained solution rather than the optimization procedure itself (although within the proposed formulation we formulate two formats for Newton-type

iterative solution of the minimization problem).

1.2 Verification and Validation

Although the concepts of *Verification* and *Validation* are more common in other areas such as software development, they play a key role in the context of the calibration of constitutive models. Babuška and Oden [3] define *verification* as the process of ensuring that the computational model can represent the mathematical model with sufficient accuracy ("Are the equations solved right?"). On the other hand, *validation* is the process of determining whether a mathematical model represents its corresponding physical event ("Are the right equations solved?"). We emphasize the difference between the mathematical model and the computational model as indicated in Figure 1.1. Calibration is in this context the proper adjustment of the mathematical model to the physical reality (in practice via experiments, which are physical models of the reality). However, in practice it is the computational model that is calibrated and, therefore, the computational model must be verified in the sense that it must be a true realization of the mathematical model. To conclude, we seek to calibrate the mathematical model, but since we can only calibrate the computational model, we must control the error between the computational and mathematical models.

In the subsequent validation step, the model predictions are compared with another *independent* set of observations of the physical reality. Again, we note that it is the mathematical model that is to be validated, but it is the computational model that is used for the predictions.

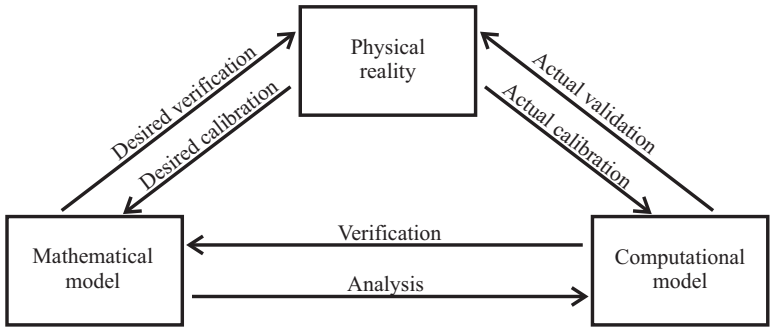

Figure 1.1: Relation between mathematical and computational models and reality.

As will be illustrated in the following example, and is also discussed by e.g Mahnken [36], successful verification and calibration do not necessarily imply a successful validation. If the different characteristics of the model are not properly activated in the experimental setup (either due to improper modeling or poorly designed experiment), the calibrated model may still produce a rather good agreement between predicted and experimental results. However, upon comparing with another (independent) experiment, we may note a

very poor agreement with the observed data that reveals the unsound choice of experiment or mathematical model.

To illustrate the importance of model validation, we consider the following example dealing with the calibration of a mechanical model for brain tissue. Experimental results from Franceschini et al. [20] show that the cerebral fluid plays an important role in the mechanical response of brain tissue for slow loading (time scale in minutes and hours). A model based on porous media theory (cf. e.g. Ehlers and Bluhm [15] for an overview of porous media theory) is employed, where the tissue is considered as a porous medium consisting of a solid skeleton with fluid- filled pores. Without going into details, the model consists of two balance laws, one for stress equilibrium (with or without acceleration terms) and another for the fluid migration following a (nonlinear) permeability law driven by the gradient of the fluid pressure. The solid skeleton is assumed to obey a viscoelastic law and a nonlinear elastic model for the bulk compressibility. The experimental setup is that of an oedometer test, as shown in Figure 1.2.

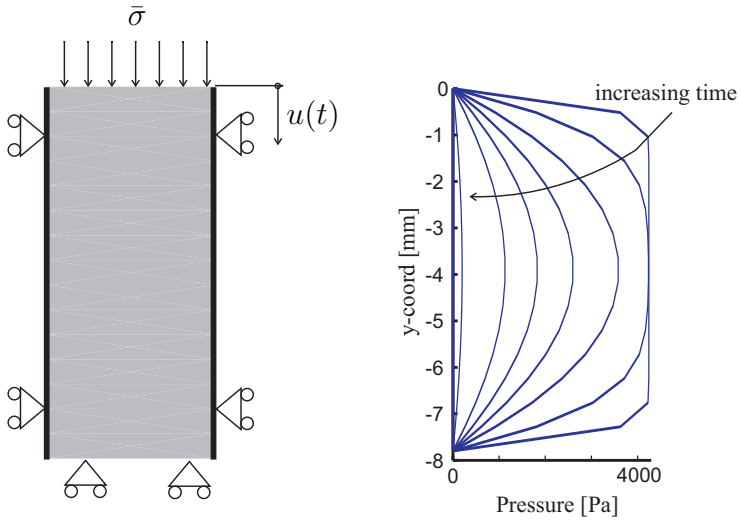

Figure 1.2: Experimental setup for oedometer test. The pressure distribution for different times is shown to the right.

A cylinder with closed walls contains the sample while the upper and lower ends are drained to allow fluid transport while retaining the solid part of the sample. The loading consists of a two-step consolidation/creep test, where a force of 3 N is applied to the upper end (leading to the prescribed stress $\bar{\sigma}$) and is held constant while the upper end displacement $u(t)$ is recorded. Initially, a pressure is built up in the fluid phase which carries the load; however, over time the fluid will migrate out of the sample through the upper and lower ends and the excess pore pressure of the fluid eventually vanishes until the prescribed stress is carried by the solid constituent only. When the displacement of the upper end has reached a stationary value (after about 200 minutes), the force is increased

with an additional 3 N and a second time-dependent response curve is obtained. The data from the fist load step is used for the calibration while the secondary load step is used for validation.

The predicted response that gives the best fit for the pertinent model is shown in Figure 1.3 together with the measured data. As can be seen (left in Figure 1.3), the model gives almost perfect fit to the data used in the calibration. On the other hand, the agreement with the data not used in the calibration (right in Figure 1.3) gives a very poor agreement, and we can conclude that the model performs poorly when it comes to validation. In the present case, the adopted model is based on the assumption of small strains, which might be an unrealistic assumption during the secondary load step. Also, the viscoelasticity properties of the solid give a rather similar response (upper end displacement) compared to the response due to the fluid migration. In fact the calibration can "hide" spurious characteristics of the chosen model, and such deficiencies can only be revealed in the validation process.

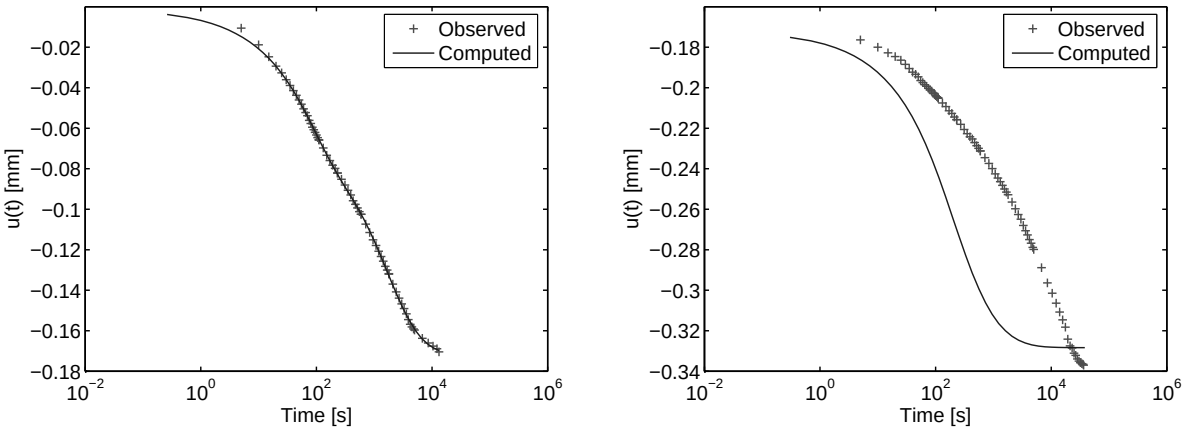

Figure 1.3: Left: Computed top end displacement after calibration. Right: Computed top end displacement for secondary loading without calibration

2 Mathematical formulation

The literature on parameter identification with a posteriori estimation of discretization errors is rather limited; however, each of the research fields known as "parameter identification" (with focus on computational algorithms and applications) and "a posteriori error estimation" (for the direct problem), taken separately, are more mature. In this section, we highlight some of the underlying ideas relevant to parameter identification with error control and give an excerpt of the relevant literature.

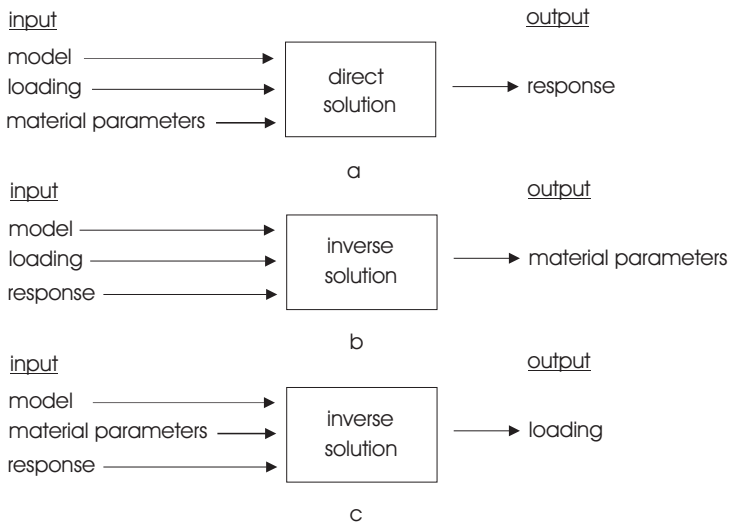

Figure 2.1: *Direct problem (a) and two subclasses of inverse problems (b,c).*

2.1 Problem formulation

We consider the general and abstract setting of a nonlinear model describing a physical/mechanical process in space-time, whose solution u depends implicitly on a parameter function p, which describes the quantity we wish to determine in the identification. The solution u is supposed to be a field in the domain Ω (in space-time) under consideration, and the nature of p depends on the specific application; p can be a set of discrete values (typically material parameters) or it can be a field in Ω. The response s is a quantity that we can observe, and it depends on p and u by a given (a priori chosen) functional relation $s = s(p, u)$. We can make a prediction of the response s for given p by solving the following equation given on variational form: Find $u(p)$ in a suitable function space $\mathbb{V}$ such that

$$a(p, u(p), v) = l(p, v) \quad \forall\, v \in \mathbb{V}^0. \tag{2.1}$$

Here, $a(p, u(p), v)$ is a semilinear form, possibly nonlinear in the two first arguments (p, u), but always linear in the last argument (v). Moreover, $l(p, v)$ is a semilinear functional (linear in v) that embodies source terms and natural boundary conditions. The computation of s for given p via the solution of (2.1) is denoted the *direct problem*, (cf. Fig. 2.1 a). Note that $u(p)$ is an *implicit* function defined by (2.1).

In contrast to the direct problem, the *inverse problem* considers the case where one (or several) of the inputs (e.g. loading or material parameters, that are described by the parameter function p) to the corresponding direct problem is unknown, whereas the response is available from experiments. In this case, we seek p in the space of admissible

parameters $\mathbb{P}$ as the minimizer to the objective function of least-squares type

$$\mathcal{F}(p, u(p)) = \frac{1}{2} \sum_{i=1}^{N^{\text{obs}}} c_i \left[s(p, u(p))(\boldsymbol{x}_i) - s^{\text{obs}}(\boldsymbol{x}_i) \right]^2 + \gamma ||p||^2 \tag{2.2}$$

where the observed response s^{obs} is measured in the points $\boldsymbol{x}_i \in \Omega, \quad i = 1, 2, \ldots N^{\text{obs}}$, and $u = u(p)$ is the solution to (2.1). Additionally, a regularization term $\gamma ||\cdot||$ of Tikhonov type can be introduced to reduce (or eliminate) the ill-posedness of the optimization problem. Issues regarding regularization are further elaborated in Section 2.3 below.

We can distinguish between two "archetypes" of inverse problems, namely (material) *parameter identification* (cf. Fig. 2.1 b) and *load identification* (cf. Fig. 2.1 c). In the former case of material parameter identification, there is typically no dependence on the sought parameter p in the loading $l = l(v)$ whereas the load identification problem has such dependence in l only (and not in a). In this thesis the main focus will be on material parameter identification, although some small steps towards the more general identification is discussed in Sections 2.3 and 6, and in Paper E.

The solution of least-squares problems governed by differential equations that requires a numerical solution strategy is a rather computationally demanding task, since the numerical solution is, typically, repeated many times as part of an iterative minimization algorithm. A general discussion of this issue can be found in Ponthot and Kleinermann [49]. In the absence of commercial tools for gradient-based optimization, there are essentially two main philosophies used in the literature. The first method to reduce computational (and implementation) time is to rely on a highly specialized (typically commercial) software for the efficient solution of the governing equation. In this case, the computation of the predicted response (to be compared to the measurement data) is treated as a "black box". Therefore, the optimization methods used are typically of the non-derivative type, such as the Nelder-Mead simplex (or an improved version called subplex, employed by Kajberg [27] in conjunction with Digital Speckle Photography to determine material parameters for steel), the response surface method employed by Omerspahic et al. [47] for determining elastic-plastic material parameters for metals, or artificial Neural Networks. In Huber and Tsakmakis [23], the considerable computational effort that is normally spent on "training" the Neural network was motivated by the possibility to reuse the same network when conducting additional experiments (using the same setup). Examples of work with focus on specific engineering analyses rather than computational aspects are the following: Bocciarelli et al. [14] calibrate hardening plasticity models using data from imprint mapping. Fedele et al. [18] study the identification of individual constituents in heterogeneous materials, taking into account the effect of noisy data. Gerlach and Matzenmiller [21] study identification problems for a certain class of viscoelastic models, whereas Tsurumi et al. [55] determine ground permeability using measurements of hydraulic head.

The alternative philosophy, that is normally more efficient than a non-derivative method and which is employed in this thesis, is to compute a derivative of the objective function in order to use a gradient-based optimization method. As will be elaborated below, the gradient and Hessian of the objective function play key roles in the subsequent error anal-

ysis. The gradient of the objective function $\mathcal{F}$ with respect to the parameter p can be obtained in two fashions, via either *direct differentiation* or by involving the *adjoint state*. A semi-analytical expression for computing the gradient is derived in the "direct differentiation" scheme put forward by Mahnken and Stein [37] and further elaborated in several publications, such as, [36], [38] and Ekh [16], Kleuter et al. [29] with explicit results for specific applications. In this scheme, an additional sensitivity field is computed by solving a differentiated version of the constitutive relation. A particular feature is that the sensitivity can be computed simultaneously as the forward solution, and it does not need to be stored, which leads to a rather efficient computation of the gradient of the objective function. The computed gradient is employed in "classical" optimization schemes, such as Gauss-Newton method or Levenberg-Marquardt, with line-search or trust-region methods to ensure convergence, as is discussed in standard textbooks such as Luenberger [35] and Fletcher [19]. Although a discussion on how the direct differentiation relates to the adjoint formulation used in this thesis can be found in Paper A, we repeat the main arguments next.

Upon differentiating $\mathcal{F}$ along the (arbitrary) direction $\delta p \in \mathbb{P}$ using the chain rule (upon treating u as a function of p), we obtain

$$\mathrm{d}_p\mathcal{F}(p, u(p); \delta p) = \mathcal{F}'_p(p, u; \delta p) + \mathcal{F}'_u(p, u; \mathrm{d}\bar{u}) \tag{2.3}$$

where $\mathrm{d}_p\bullet$ denotes a total and $\bullet'$ denotes a partial differentiation (Gâteaux-derivatives), respectively. Moreover, $\mathrm{d}\bar{u}$ is the "directional sensitivity" of the state solution u along δp, which can be computed from the differentiated (w.r.t p) version of the state equation (2.1)

$$a'_u(p, u(p), v; \mathrm{d}\bar{u}) = l'_p(p, v; \delta p) - a'_p(p, u(p), v; \delta p) \quad \forall\, v \in \mathbb{V} \tag{2.4}$$

for any $\delta p \in \mathbb{P}$. The direct differentiation method to compute the sought gradient $\mathrm{d}_p\mathcal{F}$ is, in principle, to solve (2.4) for $\mathrm{d}\bar{u}$ and insert the solution into (2.3). We note that this in practice requires p to be a set of discrete parameters rather than an arbitrary field.

In the adjoint variable method, a *costate* (sometimes also called *dual* or *adjoint*) variable λ, which resides in the test space $\mathbb{V}$, is introduced as the solution to the equation

$$a'_u(p, u, \lambda; v) = -\mathcal{F}'_u(p, u; v) \quad \forall\, v \in \mathbb{V}. \tag{2.5}$$

Now, we set $v = \mathrm{d}\bar{u}$ in (2.5) and insert the costate variable as specific test function (i.e. $v = \lambda$) in (2.4) to recast (2.3) as

$$\begin{aligned} \mathrm{d}_p\mathcal{F}(p, u(p); \delta p) &= \mathcal{F}'_p(p, u; \delta p) + \mathcal{F}'_u(p, u; \mathrm{d}\bar{u}) \\ &= \mathcal{F}'_p(p, u; \delta p) - a'_u(p, u, \lambda; v) \\ &= \mathcal{F}'_p(p, u; \delta p) + a'_p(p, u, \lambda; \delta p) - l'_p(p, \lambda; \delta p). \end{aligned} \tag{2.6}$$

We note that the costate variable λ embodies the information on how the objective function is related to the state variable. The costate variable can in this sense be interpreted as an influence function. Based on the introduction of the costate variable we can proceed

to derive the Hessian of the objective function in order obtain a Newton scheme for the optimization, which is elaborated in Laumen [34] and Paper A.

In order to determine the effect of measurement errors (i.e. noise), a sensitivity assessment can be made. Such information plays an important role in analyzing a specific experimental setup, since a large sensitivity indicates that the sought parameter depends strongly on the measured data. For the purpose of illustration, we derive a simple way to compute how the solution p to the identification problem depends on the data s^{obs}. We then consider the parameter $p = p(s^{\text{obs}})$ as a function of a specific realization of the data s^{obs} in the space of measurements $\mathbb{S}^{\text{obs}}$. Since the optimality condition

$$\mathrm{d}_p \mathcal{F}(p; \delta p) = 0 \quad \forall \delta p \in \mathbb{P} \tag{2.7}$$

must be satisfied regardless of the actual value of s^{obs}, it follows that the derivative of (2.7) with respect to s^{obs} must vanish, i.e.

$$\mathrm{d}_{s^{\text{obs}}}[\mathrm{d}_p \mathcal{F}(p, s^{\text{obs}}; \delta p); \delta s^{\text{obs}}] = 0 \qquad \forall \delta s^{\text{obs}} \in \mathbb{S}^{\text{obs}}, \forall \delta p \in \mathbb{P}. \tag{2.8}$$

Hence, we obtain

$$\mathrm{d}_{pp} \mathcal{F}(p, s^{\text{obs}}; \delta p, \mathrm{d}_{s^{\text{obs}}} p) = -\mathrm{d}_p \mathcal{F}'_{s^{\text{obs}}}(p, s^{\text{obs}}; \delta p, \delta s^{\text{obs}}) \quad \forall \delta s^{\text{obs}} \in \mathbb{S}^{\text{obs}}, \forall \delta p \in \mathbb{P} \tag{2.9}$$

and the sought sensitivity $\mathrm{d}_{s^{\text{obs}}} p$ is solved for from (2.9). The left-hand side is nothing else than the Hessian of the objective function, whereas the right-hand side is typically the derivative of the response variable $\mathrm{d}_p s$. The extension to sensitivity with respect to arbitrary quantities is elaborated further in Paper A and C, in Becker and Vexler [10] and, with application to experimental design, in Anderson et al. [2].

2.2 Finite element discretization

In standard fashion Galerkin's method is employed to solve (2.1),(2.2) numerically in space-time. We (formally) introduce the approximation spaces for the parameter and state solution, $\mathbb{P}_h$ and $\mathbb{V}_h$, respectively, although we for the case of material parameter identification often have $\mathbb{P}_h = \mathbb{P}$. The discrete version of the optimization problem (2.1),(2.2) reads: Find the minimizer $p_h \in \mathbb{P}_h$ to the objective function

$$\mathcal{F}(p_h, u_h(p_h)) = \frac{1}{2} \sum_{i=1}^{N^{\text{obs}}} c_i \left[s(p_h, u_h(p_h))(\boldsymbol{x}_i) - s^{\text{obs}}(\boldsymbol{x}_i) \right]^2 + \delta ||p_h||^2 \tag{2.10}$$

where $u_h(p_h) \in \mathbb{V}_h$ is the solution to

$$a(p_h; u_h, v) = l(p_h; v) \quad \forall\, v \in \mathbb{V}_h. \tag{2.11}$$

The discretizations defining $\mathbb{P}_h$ and $\mathbb{V}_h$ are generally different, i.e. different approximations of the parameter p and the state u are utilized. It is important to realize that the error in

u_h will affect the optimal solution p_h, even for the case of no restriction in the parameter space $\mathbb{P}_h = \mathbb{P}$. If the approximations (that are needed to solve the optimization problem in the first place) are chosen without care, the solution p_h that we obtain numerically might be a very poor approximation of the true solution p. Thus, the prime focus in this thesis is the approximation of the effect of the error $p - p_h$.

The *a posteriori* estimation discretization errors for direct problems, i.e. the effect of the error $u - u_h$ and subsequent adaptive mesh refinement, is a very active field of research. The paper by Babuška and Rheinboldt [4] is often marked as the beginning of the development of methods for a posteriori error estimation. A popular approach based on local smoothing of derivatives was put forward by Zienkiewicz and Zhu [57] and marks the start of the family of recovery-based methods. The goal-oriented approach that is used in this thesis was introduced in the 1990s, see e.g. Eriksson et al. [17]. A rather comprehensive overview can be found in Ainsworth and Oden [1]. The discussion below follows to some extent the works of Larsson et al. [31], [33].

Since the main topic of this thesis is to employ the goal-oriented approach to parameter identification problems, we shall here give a very condensed description of the main procedure for the direct problem only, while the extension to identification problems is left to the appended papers A, D and E, as well as Johansson et al. [25], [26]. In the goal-oriented approach the starting point for the error estimation is a suitably chosen *goal quantity* $\mathcal{Q}(u)$ of engineering interest that depends on the state solution u. Such quantities from the field of solid mechanics may be, e.g., the stress at some portion of the domain, or the J-integral in fracture mechanics, cf. Rüter and Stein [53], Heintz and Samuelsson [22]. In fact, the main reason that we want to use the goal-oriented approach for the identification problem is to enable the possibility to control the error in individual parameters. The estimated error is the difference in the value of $\mathcal{Q}$ between the exact and approximate solutions, i.e. the quantity $\mathcal{Q}(u) - \mathcal{Q}(u_h)$. However, we can also think of a quantity of the error directly, i.e. $\mathcal{Q}(u - u_h)$ to accommodate the case when the quantity of interest is typically some norm of the error.

We recall the previous discussion on how a costate problem could be used to relate a change in the state solution to the objective functional, (2.6). The same idea is used here to relate the error ("change") in the state solution to the goal quantity $\mathcal{Q}$, such that the estimate of the error in $\mathcal{Q}$ is obtained by weighting the finite element residual $\mathcal{R}(u_h, v) \stackrel{\text{def}}{=} l(p, v) - a(p, u_h, v)$ with the dual solution u^* as follows:

$$\mathcal{Q}(u) - \mathcal{Q}(u_h) = \left[\hat{\mathcal{Q}}'_u(u, u_h; e) = \hat{a}'_u(u, u_h; u^*, e) = \right] \mathcal{R}(u_h, u^*). \tag{2.12}$$

Here, we introduced the error $e \stackrel{\text{def}}{=} u - u_h$ and the secant forms

$$\hat{\mathcal{Q}}'_u(u, u_h; w) \stackrel{\text{def}}{=} \int_0^1 \mathcal{Q}'_u(u_h + se; w)\mathrm{d}s = \mathcal{Q}(u) - \mathcal{Q}(u_h) \tag{2.13}$$

$$\hat{a}'_u(u, u_h; \delta u, w) \stackrel{\text{def}}{=} \int_0^1 a'_u(p, u_h + se; \delta u, w)\mathrm{d}s = a(p, u, v) - a(p, u_h, v) = \mathcal{R}(u_h, v). \tag{2.14}$$

Thus, the error estimate requires the solution of a dual problem on secant form: Find $u^* \in \mathbb{V}^0$ such that

$$\hat{a}'_u(u, u_h; u^*, \delta u) = \hat{\mathcal{Q}}'_u(u, u_h; \delta u) \quad \forall \delta u. \in \mathbb{V}^0. \tag{2.15}$$

In principle, we have the Galerkin orthogonality property, i.e. $\mathcal{R}(u_h, v) = 0$ for any $v \in \mathbb{V}_h^0$, which in practice is not satisfied due to inexact solution of the discretized state equation (e.g. termination of iterative solution, rounding errors). We split the error representation into two contributions, discretization and solution error, respectively, by subtracting an interpolant $\pi_h u^* \in \mathbb{V}_h^0$

$$\mathcal{Q}(u) - \mathcal{Q}(u_h) = \mathcal{R}(u_h, u^*) = \underbrace{\mathcal{R}(u_h, u^* - \pi_h u^*)}_{\text{Discretization}} + \underbrace{\mathcal{R}(u_h, \pi_h u^*)}_{\text{Solution}}. \tag{2.16}$$

An important property of the error representation (2.16) is that it is *exact* provided that u^* is the exact solution of the dual problem (2.15). Unfortunately, the exact solution is inaccessible since the secant forms, cf. (2.13),(2.14), requires knowledge of the exact solution u, which we do not have, and, additionally, is infinite-dimensional. The common approach is to linearize the secant forms at the solution u_h, thus obtaining the corresponding (linear) tangent forms, and introduce an FE-approximation of the dual variable denoted $\tilde{u}_h^*$. Hence, (2.15) is recast as: Find $\tilde{u}_h^* \in \tilde{\mathbb{V}}_h^0$ such that

$$a'_u(u_h; \tilde{u}_h^*, \delta u) = \mathcal{Q}'_u(u_h; \delta u) \quad \forall \delta u \in \tilde{\mathbb{V}}_h^0 \tag{2.17}$$

The introduction of the tangent forms provides a direct estimation of the actual error, but unfortunately, without specific bounds. As a result of the Galerkin orthogonality the dual solution $\tilde{u}_h^*$ cannot reside in the discrete space $\mathbb{V}_h$, i.e. we cannot have $\tilde{\mathbb{V}}_h^0 = \mathbb{V}_h^0$. Here, a typical trade-off between accuracy and computational effort arise: The richer we choose $\tilde{\mathbb{V}}_h^0$, the more accurate the error estimation will be, but also the more computational work will be needed. A simple, but still rather computationally demanding approach, is to solve the dual problem (2.17) using one higher order basis functions (p-refinement, in contrast to h-refinement where additional elements are added) for $\tilde{\mathbb{V}}_h^0$. If a hierarchial basis is chosen it is possible to solve (2.17) for the added part $\Delta\tilde{\mathbb{V}}_h^0 = \tilde{\mathbb{V}}_h^0 \setminus \mathbb{V}_h^0$ only, which is considerably cheaper than solving the fully expanded system (2.17) for $\tilde{\mathbb{V}}_h^0$, cf. Larsson et al. [31]. Another approach is to solve the dual problem (2.17) in $\mathbb{V}_h$, and then construct the solution in $\tilde{u}_h^*$ using some post-processing scheme, cf. Larsson et al. [33].

The use of goal-oriented methods are rather widespread. For instance, Prudhomme and Oden [50] derive upper and lower bounds for the estimate along with a technique to construct goal quantities for pointwise errors, even at points where the state solution may not be continuous, using averaging functions ("mollification"). Another idea for the formulation of the goal-oriented approach is to consider enhancement of both the primal and dual solution, yielding the "optimal control"-approach put forward by Becker and Rannacher [8]. Although the enhancement of the primal solution requires additional computational effort, the error estimate is second order accurate.

The estimated error is often used to provide feedback for the subsequent adaptive mesh-refinement, either by changing the mesh-size (h-refinement) or the polynomial of the basis

functions (p-refinement). In such methods, the error representation (2.12) is localized to element contributions, and typically those elements that give the largest contributions are split in smaller elements in order to get accurate solutions at low computational cost. Discussion on refinement strategies can be found in Rannacher [51], Larsson et al. [32].

To conclude the discussion on a posteriori error estimation and adaptivity based on the pertinent dual problem for the direct problem, we refer the reader to the Ph.D theses of Larsson [30] and Rüter [52] and references therein.

The literature on the extension of the concept of goal-oriented error estimation to the calibration problem is limited to the group around Becker and Vexler, apart from the present thesis and the work of Beilina et al. [11] [12] which is discussed in Section 2.3 below. In the thesis of Vexler [56], proofs regarding existence and uniqueness of the identification problem is given, along with aspects on optimization methods and error estimations following the "optimal control" approach [8]. Other works of Becker and Vexler include applications to stationary problems, with applications in fluid dynamics [10] and convection-diffusion problems [9], in combustion [6], and extension to time-dependent problems [41], [7]. Those works apply the "optimal control" approach for the error computation, thus ending up with six fields (parameter, state and costate, and corresponding dual fields) whose enhancements are weighted together to give a second order accurate error estimation. In contrast to the "optimal control" approach, we retain in this thesis (as does Beilina et al. [11], [12]) the simpler procedure outlined above to obtain a first order accurate estimate of the error.

2.3 The case of parameters as arbitrary functions

An important aspect of an inverse problem is the nature of the sought parameters p. In the case when p represents a set of discrete values, such as distinct material parameters in a given constitutive model, it is reasonable to expect that the optimization problem is well-posed, which is in sharp contrast to the case where p represents an (arbitrary) function. The latter case is what is usually thought of when inverse problems are judged as being ill-posed. Examples of problems where p represents an (arbitrary) function is the load identification problem mentioned above, where p is a sought load history, which for the linear case has received considerable attention, e.g. Trujillo and Busby [54], Nordström [45], Nordberg and Gustafsson [43], [44]. In Paper E, p represents a sought distribution function that defines a class of viscoelastic material models. Another relevant application is the identification of inhomogeneities from wave reflection data, for instance with application to acoustics and microscopy, see Beilina et al. [11] [12].

The ill-posedness of the identification problem is often due to instability in the sense that the solution does not depend continuously on the data. A small perturbation of the measured data can give rise to a totally different optimal solution (cf. Nordberg [42]), and such perturbations are always present in numerical computations (e.g. round-off errors). The instability is often manifested as extensive oscillations in p, and the standard method to obtain a more "pleasing" solution (from an engineering point of view) is to add

regularization. Normally, a heavily oscillatory solution is not realizable in practice, and it is therefore commonly accepted to add a priori information in terms of a penalty factor (cf. (2.2)) of a norm of p or its derivative (Tikhonov regularization). Clearly, the proper weighting between the least-squares part and the penalty term in the objective function controlled by γ is crucial for the outcome. A similar difficulty with oscillatory parameter solutions ("checkerboard") arises in the closely related shape and topology optimization problems, as discussed in Bendsøe [13], Jog and Haber [24], Petersson [48].

An important observation made in Nordström et al. [46] and Paper E is that, although the continuous problem (2.1),(2.2) is severely ill-posed, its discrete version (2.10),(2.11) can be somewhat less ill-posed. In fact, the choice of $\mathbb{P}_h$ can be considered as a sort of *a priori* regularization, where a finer discretization leads to increasing ill-posedness. Obviously, there is a trade-off between errors from the discretization and errors due to extensive regularization controlled by γ. A posteriori error estimation and adaptivity for inverse problems is discussed in Beilina et al. [11], [12], and a scheme for controlling discretization and regularization errors is outlined by Bangerth [5].

3 Practical use of the proposed methodology

3.1 Commercial software

The practical applicability of error-controlled parameter identification depends on how well such procedures can be implemented or combined with widespread (often commercial) finite element softwares. As briefly mentioned in Subsection 2.2 above, the costate problem (2.5) plays an integral part in the proposed formulation. To the author's knowledge, out of the major commercial FE software used in industry (e.g. Abaqus, LS-Dyna, Diana, Radioss), there is none that has implemented a posteriori error computation based on a dual problem, which is likely due to the large memory requirement (in principle, the full time-history of the state solution needs to be stored) and computational efforts involved. Since the costate problem (2.5) is very similar to the dual problem (2.17) used for the error computation for the direct problem, it is unlikely that the methodology discussed in this thesis will be implemented in full in commercial FE-software in the near future.

In most practical engineering situations, the user has to resort to the "black-box" approach, mentioned in Section 2.1 above. A general purpose optimization software with a specialized FE-solver is used such that, for the evaluation of the objective function, the optimization program calls the FE-solver for a specific input (p), and the output u of the solver is processed to extract the predicted response s. In fact, optimization features that exist in some commercial FEM packages often use the black-box approach (e.g. LS-Opt). Although the formal a posteriori error computation in such an approach is inaccessible, it may in practice be sufficient to perform a simple convergence study, i.e. monitoring how much the parameters, objective function and other quantities of interest change for a series of refined FE-meshes. The simplified sensitivity assessment mentioned in Section 2.1 above can actually be computed using finite difference computation of the pertinent derivatives

and Hessian. The computed derivatives can subsequently be used to obtain a correlation matrix (cf. Paper C, Ekh [16]) to reveal interdependencies between different parameters. With the aid of sensitivity assessment and convergence studies, the most important sources of errors can be investigated, including noise in data and discretization errors.

A remark regarding the practical implementation of the full error-controlled identification procedure is warranted: A closer look at the costate problem (2.5) reveals that the right-hand side is nothing else than a particular set of point loads acting at the measurement points, while the left-hand side is a linearization at the solution point, which is nothing else than the last stiffness matrix in a Newton procedure. Thus, the re-coding effort to include the solution of the pertinent costate problem is limited; however, assembling the gradient and computation of the components in the Hessian matrix is a much more complicated task.

3.2 Connection to probabilistic analysis

An important "customer" of error-controlled identification is the field of probabilistic analysis. In contrast to deterministic analysis, the simulation predictions are expressed in terms of statistical measures (e.g. mean, variance). Probabilistic analysis has become an increasingly important tool in engineering practice cf. Matthies et al. [39], [40], Kleiber [28], to meet the increasing demand for quality-assurance. Such analyses, also referred to as probabilistic design, are particularly important in structural engineering applications (e.g. analysis of houses, bridges, ships, etc.). The outcome of the error computation and sensitivity assessments for the parameter identification serves as input for the subsequent probabilistic analyses where the identified parameters are used.

4 Contributions compared to available literature

As seen in Section 2.2 above, much of the mathematical framework can be found elsewhere; however, it is the work of Becker and Vexler (and coworkers) which is most closely related. It is essentially only this group that deals with error estimation and sensitivity assessment in conjunction with parameter identification in a similar fashion as discussed in this thesis. In a broader sense; however, this thesis gives strong support to the work of Becker and Vexler [10].

The work in the present thesis is (to the author's knowledge) novel in the following respects:

- A specific a posteriori error estimation method (following Larsson et al. [31]) is extended to parameter identification problems. The used method is similar to the one put forward by Becker and Vexler [10], since both are based on the appropriate dual problem. However, the actual error computations are different.
- In contrast to the papers by Becker and Vexler (and coworkers), the focus is on applications in computational solid mechanics.

- It is shown how the time-flow structure of the pertinent state equation can be utilized to obtain a computational scheme for the Newton system.
- A comparison of different (time)mesh-refinement strategies for a parameter identification problem, particularly with respect to several goal quantities simultaneously, is made in Paper D.
- The effect of model errors, treated as approximation errors in the parameters, is investigated in Paper E and [25].
- It was demonstrated that the parameters related to viscous effects in the Bergström-Boyce model are sensitive to measurement errors when calibrated against uniaxial test data at quasi-static conditions.
- The determination of the diffusion coefficient in wood using indirect measurement of the moisture content profile in combination with a parameter identification technique gives a more robust scheme than traditional techniques based on direct measurement of moisture transport through a thin wood sample.

5 Summary of appended papers

In **Paper A**, *Parameter identification with sensitivity assessment and error computation*, the general format for a posteriori error estimation is outlined, along with the corresponding "direct differentiation" format put forward by [37]. The direct and the dual method for computing sensitivity assessments are outlined.

In **Paper B**, *Numerical determination of diffusion coefficients in wood using data from CT-scanning*, a deeper look at a specific application is taken. Here, the framework is used for the determination of the diffusion coefficient in wood. A wood sample is dried in a climate chamber while the time-history of the moisture content profile is obtained using a Computer Tomography in conjunction with Digital Speckle Photography. Although not explicitly reported, a convergence study showed that the discretization errors could be neglected compared to effects of noise in the data.

In **Paper C**, *Calibration of a class of nonlinear viscoleasticity models with sensitivity assessment based on duality*, the time-flow structure is utilized to obtain a practical computational scheme. In particular, it was shown how the sensitivity in the parameters with respect to measurement noise can be computed and used to quantify the effect of a particular noise. In the case of actual experimental data under quasi-static loading, the parameters related to the viscous feature in the Bergström-Boyce model was very sensitive to measurement errors.

Paper D, *Calibration of a class of nonlinear viscoelasticity models with adaptive error control*, is a continuation of Paper C. A posteriori error computation is used as feedback for adaptive (time)mesh-refinement in order to reduce the discretization error below a chosen tolerance. The tolerance is chosen based on the influence of measurement errors such that

the time-mesh is locally refined until the estimated discretization error is small compared to the errors due to measurement noise. Four adaptive mesh-refinement strategies are compared. Additionally, a computationally cheaper procedure for computing the error estimation based on local enhancement of the dual solution was tested and found to be working satisfactorily.

In **Paper E**, *Estimation of model errors in the calibration of viscoelastic material models*, the error introduced due to the choice of parameter discretization is examined. The errors arising from a discretization of the parameter space $\mathbb{P}_h \subset \mathbb{P}$ are treated in the same manner as the "classical" errors due to the discretization of the state space $\mathbb{V}_h \subset \mathbb{V}$. For the case of determining a distribution function describing the viscoelastic relaxation spectrum, it was found that the identification problem became increasingly ill-posed for finer discretizations.

6 Concluding remarks and future work

A method for a posteriori error computation and sensitivity assessment for identification problems has been developed and tested in various examples. The procedure gives reasonable results in terms of the quality of the error estimation; however, all the considered examples are far too simple to allow for definite conclusions regarding the overall performance. The practical implementation in commercial software is still many years ahead, but in the meantime so-called black-box schemes based on finite difference computation of derivatives and convergence studies can be very useful tools in analyzing the solution of parameter identification problems.

In the short perspective, one course for further research is to focus more on real engineering problems including actual test data. For instance, a combination of Paper C (real data) and Paper D (adaptive mesh-refinement) seems tractable. Also, a full space-time adaptive mesh-refinement scheme can be tested for the wood drying problem in Paper B. An additional important field is that of biomechanics, which has gained a very large attention in the mechanics community in recent years. In contrast to classical engineering materials like steel, biological materials involve a number of complex phenomena such as different in vitro vs. in vivo properties, anisotropy and highly nonlinear response, self-activation through chemical and electrical stimuli. On top of that, there is often a huge scatter in the data which may be attributed to significant variation between different samples.

In the longer perspective, another course of research is error-controlled inverse identification including adaptive regularization. In this case we pursue the direction of Paper E and Section 2.3 above, where the sought parameter p is an arbitrary function. A particular problem is that the solution of the continuous problem is unstable in the general case, and a suitable regularization is needed. Although the discretized problem has a stable solution, we cannot expect convergence for increased mesh-refinement. This complication poses interesting challenges for the performance of the a posteriori error estimation.

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Appended Papers A-E

Paper A

Parameter identification with sensitivity assessment and error computation

H. Johansson, K. Runesson and F. Larsson
GAMM Mittelungen **30**, 430–457 (2007).

Paper B

Numerical determination of diffusion coefficients in wood using data from CT-scanning

J. Eriksson, H. Johansson and J. Danvind
Wood and Fiber Science **38**, 334–344, (2006).

Paper C

Calibration of a class of nonlinear viscoleasticity models with sensitivity assessment based on duality

H. Johansson and K. Runesson
International Journal for Numerical Methods in Engineering **69**, 2513–2537, (2007).

Paper D

Calibration of a class of nonlinear viscoelasticity models with adaptive error control

H. Johansson, K. Runesson and F. Larsson
Published online in *Computational Mechanics*, doi: 10.1007/s00466-007-0172-z (2007).

Paper E

Estimation of model errors in the calibration of viscoelastic material models

H. Johansson, F. Larsson and K. Runesson
To be submitted for publication